seqabc

December 15, 2021

approximate bayesian computation

[1]:
```
import sys, os
import copy
join = lambda *x: os.path.abspath(os.path.join(*x))
import numpy as np
import matplotlib.pyplot as plt
import matplotlib as mpl
import pandas as pd
import seaborn as sns
import scipy.stats

import pili
import parameters
import _fj
import fjanalysis
import twanalyse
import rtw
import sobol
import abcimplement
from abcimplement import mirror, mirrorpts
```

```
WARNING: did not find local config.txt, default params loaded
```

[ ]:
```

```

[2]:
```
verbose = False
style = {}
```

[3]:
```
notedir = os.getcwd()
root = pili.root
# candidate to compare against
# simdir = join(root, "../run/5bfc8b9/cluster/mc4d")
simdir = join(root, "../run/825bd8f/cluster/mc4d")
```

[4]:
```
# load fanjin data
all_idx, ltrs = _fj.slicehelper.load_linearized_trs("all")
reference_idx = _fj.load_subset_idx()
```

```
subsets = list(reference_idx.keys())
```

```
100%|     | 3113/3113 [00:01<00:00, 2338.97it/s]
```

[5]:
```
mc4d = {}
mc4d["simdir"] = simdir
objectives = ['lvel.mean', 'deviation.var', 'qhat.estimate', 'ahat.estimate']
mc4d["objectives"] = objectives
abcimplement.load_problem_simulation(mc4d)
lookup = mc4d["lookup"]
problem = mc4d["problem"]
lduid = mc4d["lduid"]
```

```
nan found in lvel.mean. filtering 1 samples
nan found in deviation.var. filtering 1 samples
nan found in qhat.estimate. filtering 1 samples
nan found in ahat.estimate. filtering 1 samples
failed: Counter({'step_condition': 1})
filtered out 1/10000 samples
loaded data from  /home/dan/usb_twitching/run/825bd8f/cluster/mc4d
```

[6]:
```
# velocity similarity scores are summary statistics that are
# already computed against the reference data
# We need to handle them differently
ks_scores = ['fanjin.%s.ks_statistic' % subset for subset in reference_idx.
 ↪keys()]

print("objectives", objectives)
_data =  sobol.collect_obs(lookup, lduid, objectives, objectives)
missing = sobol.check_missing(lookup, _data)
print(missing)
```

```
objectives ['lvel.mean', 'deviation.var', 'qhat.estimate', 'ahat.estimate']
None
```

[7]:
```
refdf = fjanalysis.compute_reference_data(ltrs, reference_idx, objectives)
```

```
/home/dan/usb_twitching/pili/src/analysis/twanalyse.py:957: RuntimeWarning:
invalid value encountered in true_divide
  norm_dy = dy/np.linalg.norm(dy, axis=1)[:,np.newaxis]
```

[8]:
```
# construct data frame with parameters and objectives
params = mc4d["data"].paramsdf(objectives)
params
```

[8]:
```
             uid  dwell_time    pilivar  anchor_angle_smoothing_fraction  \
0    _u_Ggkp1Yqv    0.277358   2.972168                         0.636124
1    _u_kO2vLVPq    2.290156  13.458395                         0.982386
```

```
2     _u_f07f6w1e    1.152016   4.898614                        0.791042
3     _u_5x7UXRa3    2.895285   9.772801                        0.601714
4     _u_xD799B4g    2.235726  14.043213                        0.804412
…          …          …         …                          …
9994  _u_q7T1w8MB    0.517194   6.952505                        0.678124
9995  _u_pR5a08wh    2.703825  12.438112                        0.360815
9996  _u_gYAqb1Pd    2.004187   2.643347                        0.428564
9997  _u_4q0YoFeA    0.810165  13.788433                        0.252809
9998  _u_WMZ8jTmp    0.977512  13.887472                        0.145301

       k_spawn  lvel.mean  deviation.var  qhat.estimate  ahat.estimate
0     4.200050   0.111104       0.612706       0.444574       0.332158
1     4.910491   0.220407       0.485135       0.682960       0.374695
2     3.650944   0.172579       0.567951       0.602694       0.367633
3     5.800258   0.187449       0.622302       0.629465       0.321893
4     2.256907   0.109917       0.196990       0.713616       0.307400
…        …          …            …              …              …
9994  6.057240   0.179546       0.287126       0.610588       0.339045
9995  1.686277   0.067876       0.157684       0.653821       0.226175
9996  4.048677   0.121132       0.855941       0.531354       0.287960
9997  5.810044   0.090522       0.110491       0.607698       0.201815
9998  7.280983   0.057255       0.105679       0.486746       0.165886

[9999 rows x 9 columns]
```

[9]:
```
# similar for ks_statistic
_parlist = list(zip(problem["names"],  zip(*[lookup[1][_u] for _u in␣
 ↪lookup[0]])))
_col = {k:v for k, v in _parlist}
_data =  sobol.collect_obs(lookup, lduid, ks_scores, ks_scores)
_col.update({name:_data[name] for name in ks_scores})
ksparams = pd.DataFrame(_col)

for score_subset in ks_scores:
    print("{} min = {:.4f}".format(score_subset, ksparams[score_subset].min()))
```

```
fanjin.candidate.ks_statistic min = 0.1817
fanjin.top.ks_statistic min = 0.0956
fanjin.half.ks_statistic min = 0.0969
fanjin.median.ks_statistic min = 0.0382
fanjin.walking.ks_statistic min = 0.0708
```

[10]:
```
# plot the sampling distribution (uniform random)
# any projection will do
if verbose:
    plt.rcParams.update({'text.usetex': False})
    fig, ax = plt.subplots(figsize=(5,5))
```

```
    sns.scatterplot(params["pilivar"],␣
↪params["anchor_angle_smoothing_fraction"],
        hue=params["ahat.estimate"], ax=ax)
```

[11]:
```
# Implement rejection ABC
# we can construct an approximate posterior distribution for
# 1. simulated reference
# 2. fanjin data subsets
from abcimplement import rejection_abc
parnames = problem["names"]
bounds = problem["bounds"]

# select the "top" subset as the preferred reference data
subset = "top"
reference = refdf.iloc[1]
```

[12]:
```
# construct a dictionary of dataframes, one for each summary statistic we will␣
↪use
accept  = {}
N = 200
for objective in objectives:
    statdf = params[parnames+[objective]]
    accepted = rejection_abc(statdf, [objective], reference, N)
    # max_score = accepted.iloc[N-1]["score"]
    # print("max score is", max_score)
    accept[objective] = accepted

# add the lvel similarity stat
top_ks = "fanjin.top.ks_statistic"
ks_statdf = ksparams[parnames+[top_ks]]
accept[top_ks] = rejection_abc(ks_statdf, [top_ks], reference, N)
```

```
['lvel.mean']
(9999, 1)
['lvel.mean']
N = 200, delta = 0.0023010600373943035, target = [0.07223161]
['deviation.var']
(9999, 1)
['deviation.var']
N = 200, delta = 0.022738550548110026, target = [0.70864216]
['qhat.estimate']
(9999, 1)
['qhat.estimate']
N = 200, delta = 0.002859086534804045, target = [0.57221674]
['ahat.estimate']
(9999, 1)
['ahat.estimate']
```

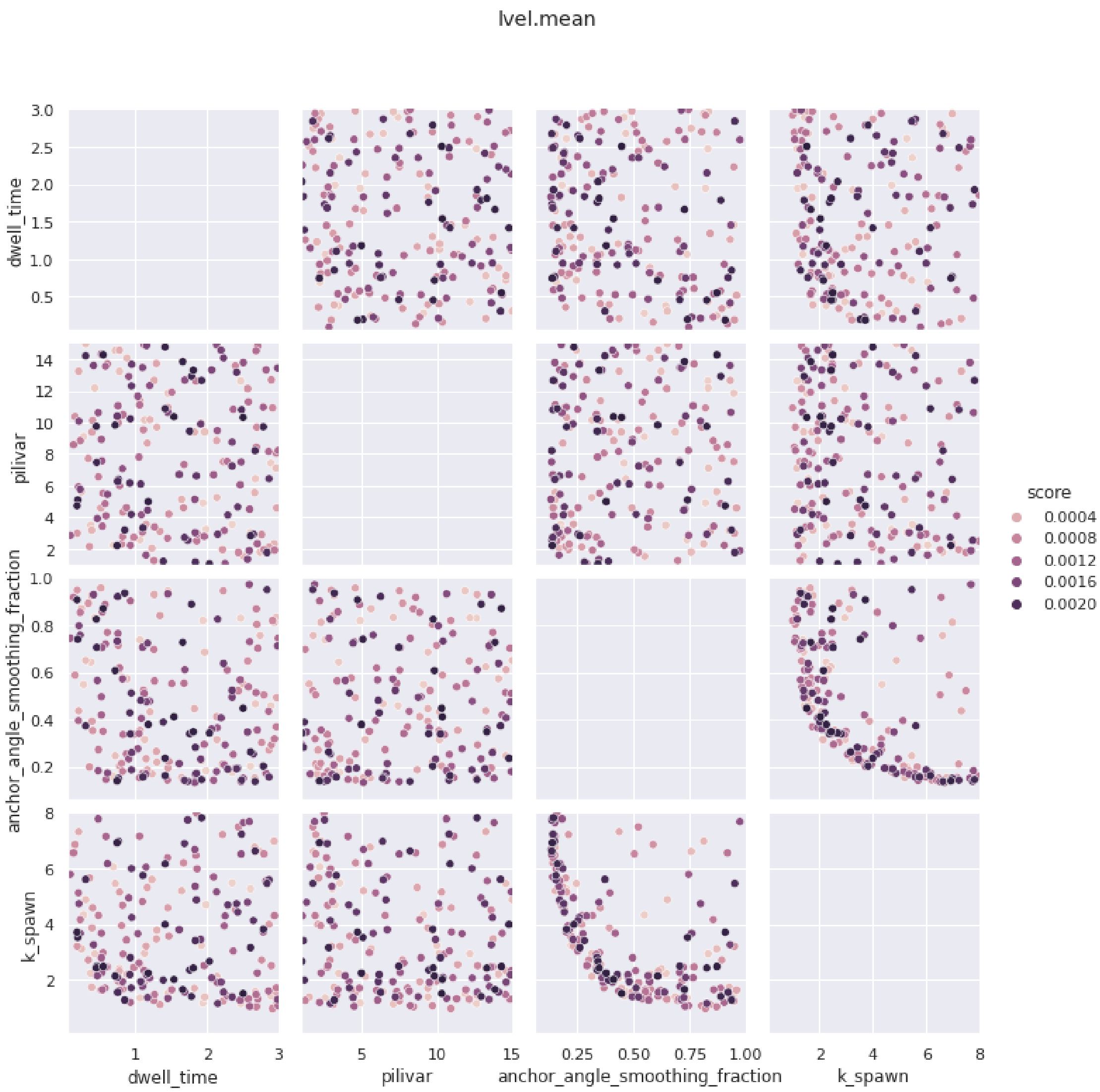
```
N = 200, delta = 0.011243760546231815, target = [0.08248354]
['fanjin.top.ks_statistic']
(9999, 1)
['fanjin.top.ks_statistic']
N = 200, delta = 0.1948867758811624, target = [0.]
```

```
/home/dan/usb_twitching/pili/src/analysis/abcimplement.py:129:
SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  statdf["score"] = score
```

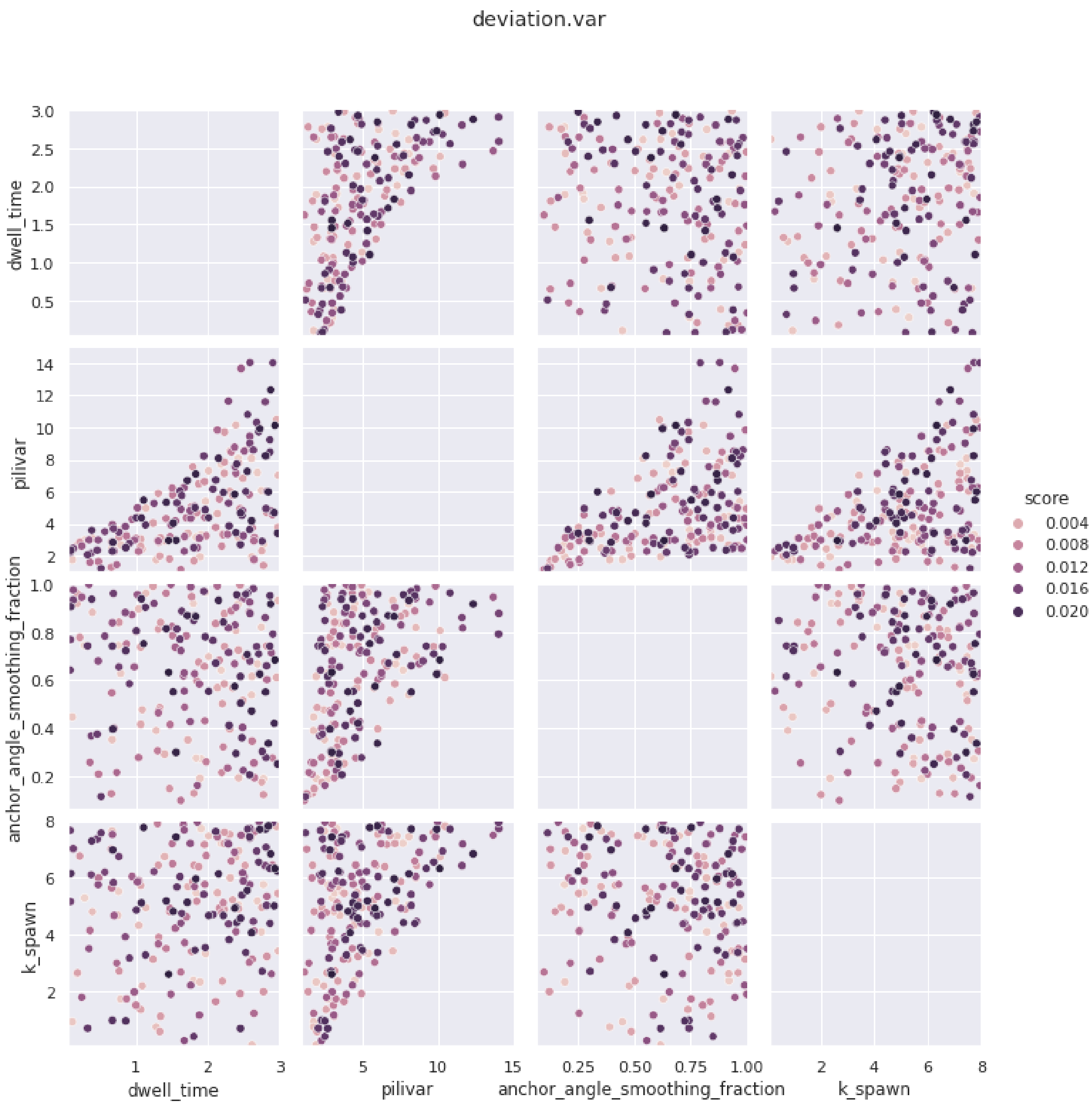
[13]:

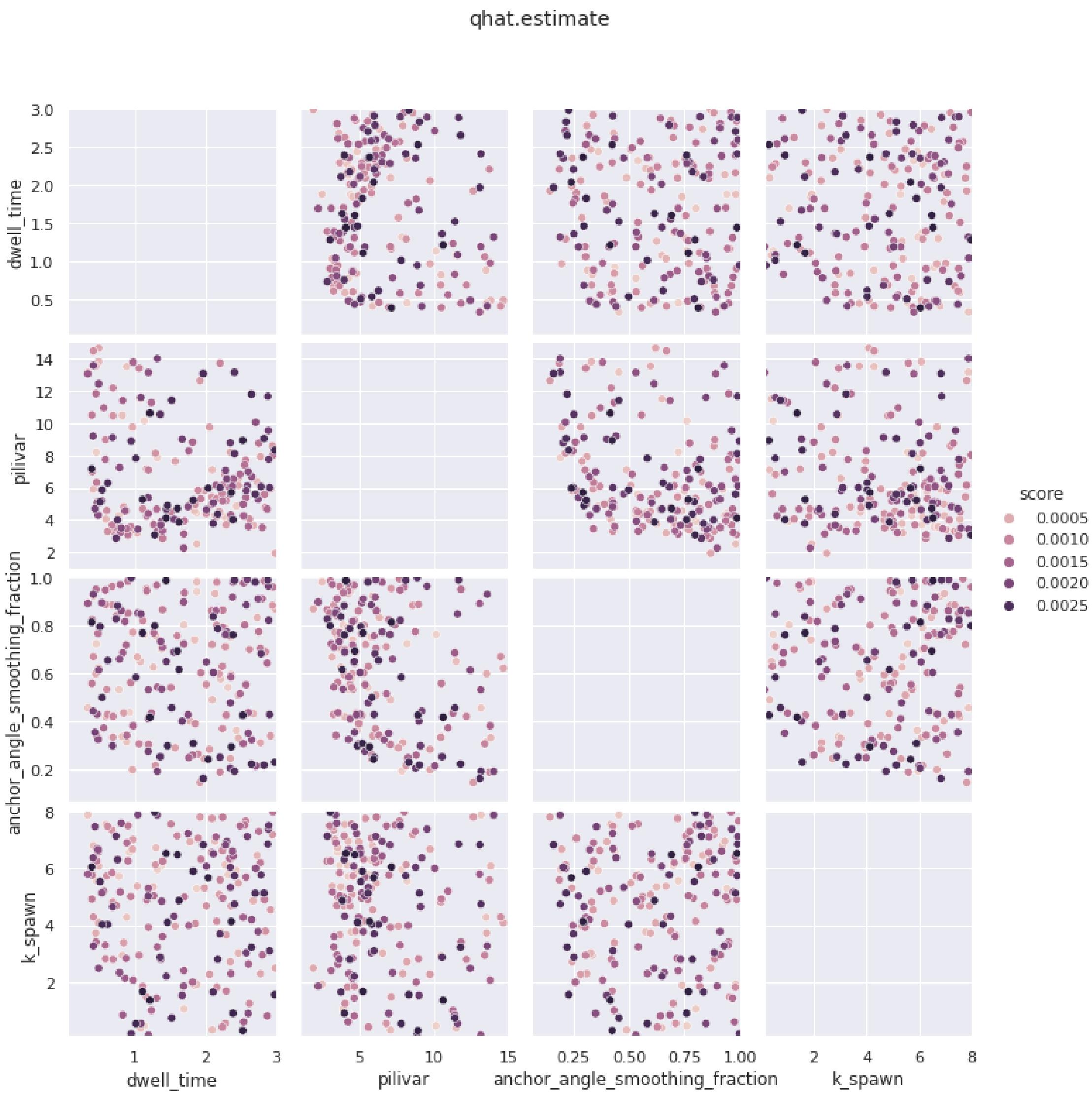
```
# show the rejection_abc results in all pairs of dimensions
n = len(problem["names"])
plt.rcParams.update({'text.usetex': False})
sns.set(rc={'figure.figsize':(20,20)})
print("plotting pairplots for ", list(accept.keys()))
for objective, accepted in accept.items():
    # print(objective)
    is_lvel = objective.startswith("fanjin")
    if is_lvel:
        data  = accepted[parnames+[objective]]
        hue = objective
    else:
        data  = accepted[parnames+["score"]]
        hue = "score"
    g = sns.pairplot(data, hue=hue, **style)
    g.fig.suptitle(objective, y=1.08) # y= some height>1
    for i in range(n):
        for j in range(n):
            if i==j:
                continue
            _xlim = bounds[j]
            _ylim = bounds[i]
            g.axes[i,j].set_xlim(_xlim)
            g.axes[i,j].set_ylim(_ylim)
```

```
plotting pairplots for  ['lvel.mean', 'deviation.var', 'qhat.estimate',
'ahat.estimate', 'fanjin.top.ks_statistic']
```

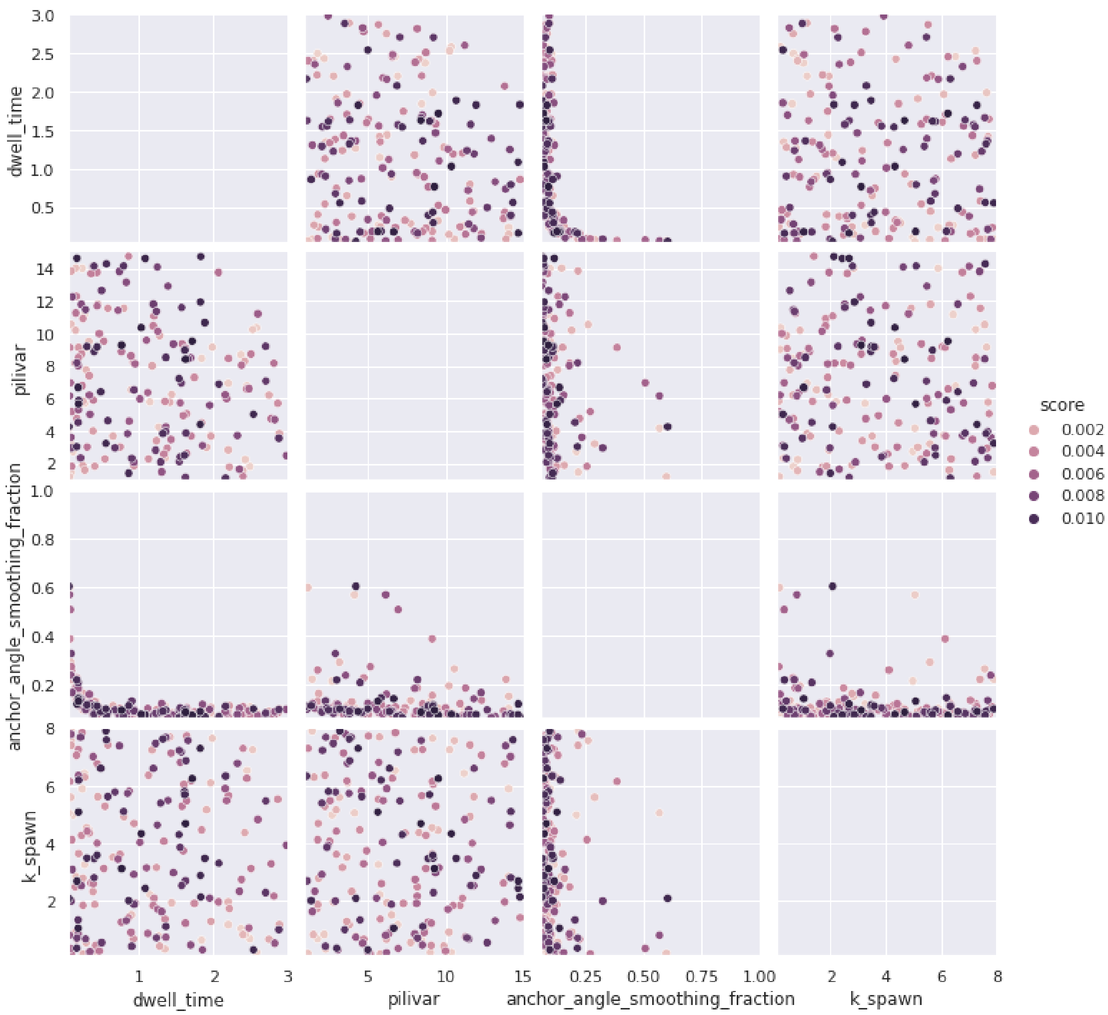


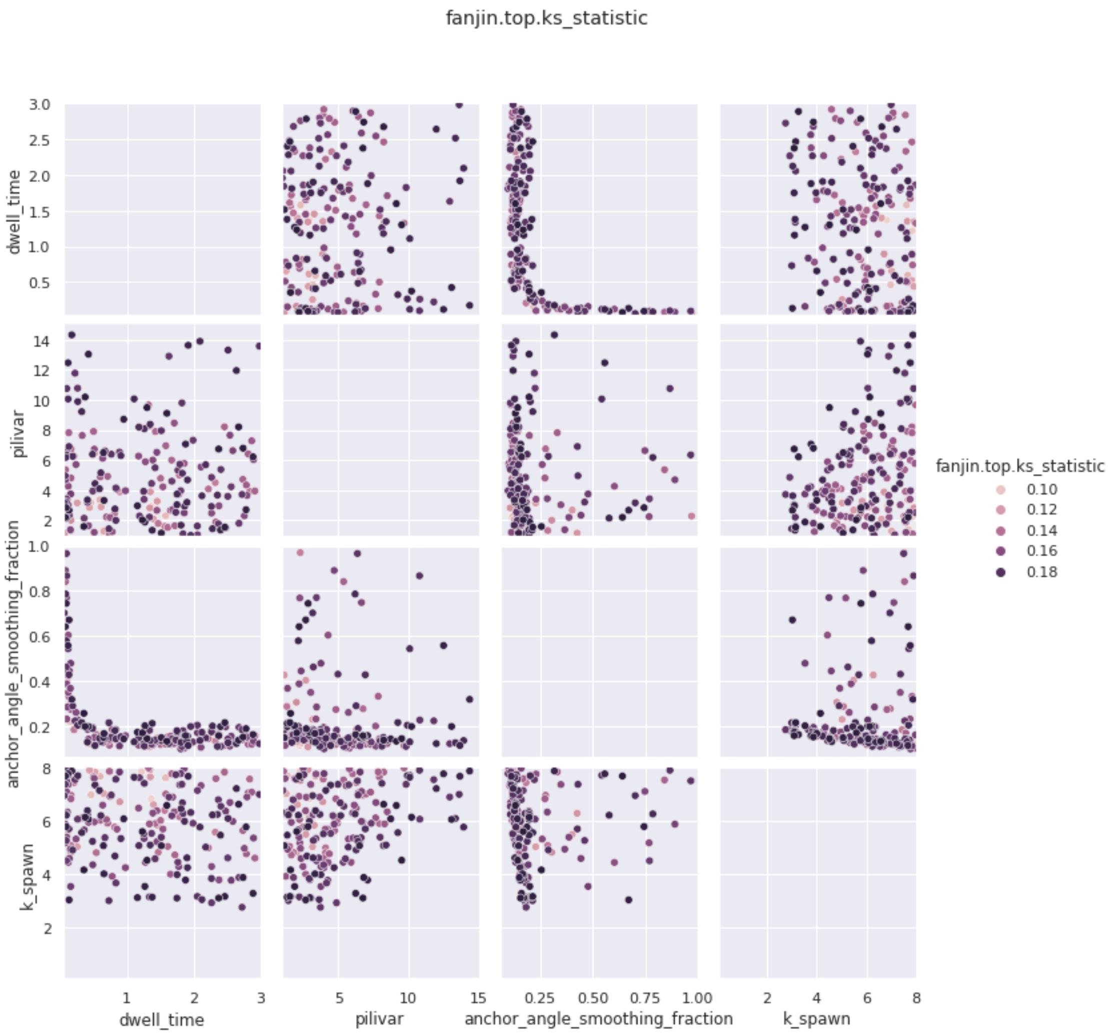
lvel.mean
dwell_time
pilivar
anchor_angle_smoothing_fraction
k_spawn
score
0.0004
0.0008
0.0012
0.0016
0.0020


deviation.var
dwell_time
pilivar
anchor_angle_smoothing_fraction
k_spawn
score
0.004
0.008
0.012
0.016
0.020


qhat.estimate
dwell_time
pilivar
anchor_angle_smoothing_fraction
k_spawn
score
0.0005
0.0010
0.0015
0.0020
0.0025

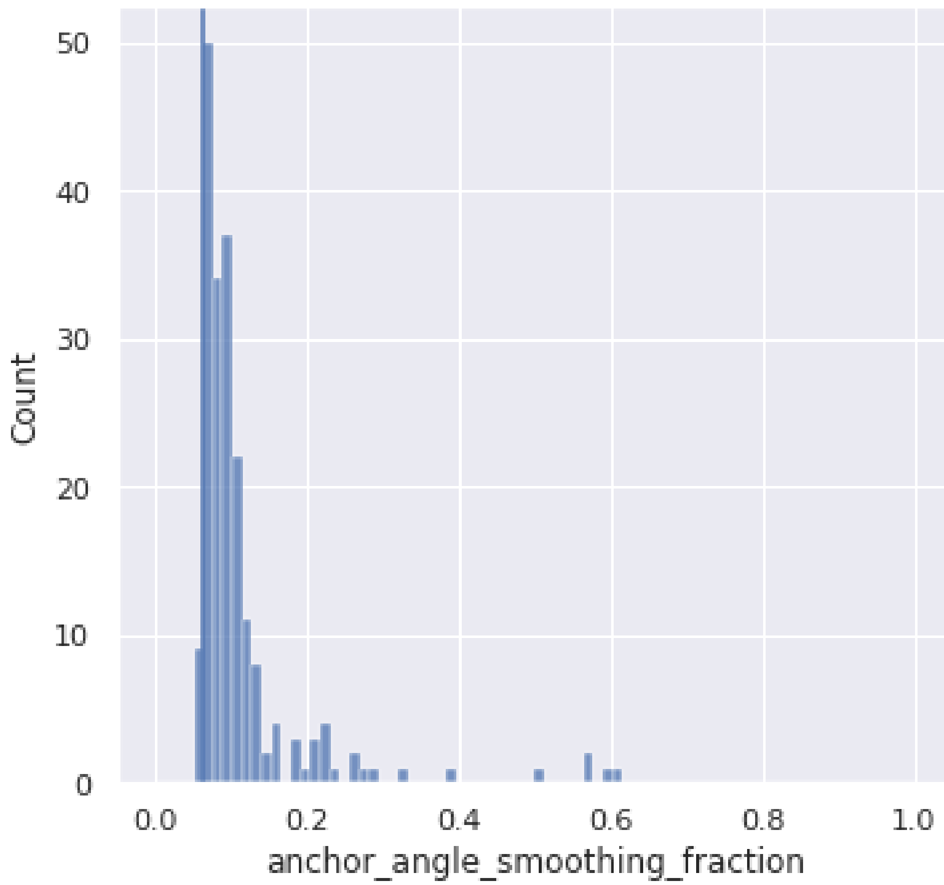
ahat.estimate

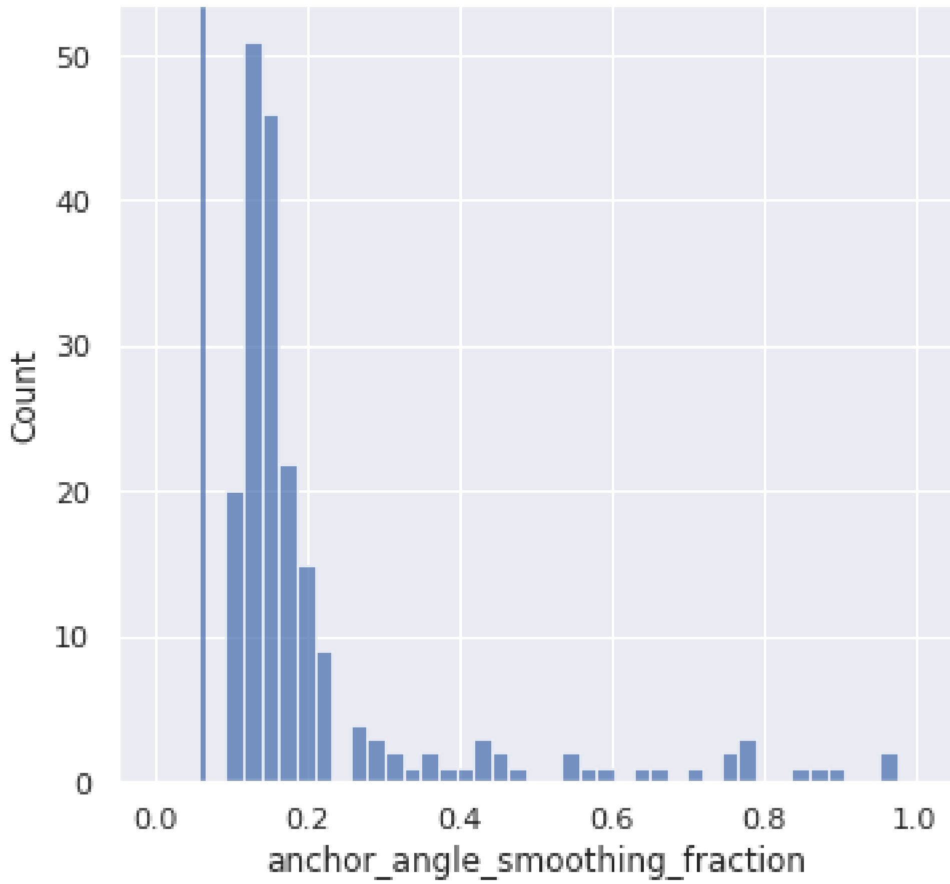




[14]:
```
# pull estimates for anchor parameter for "top" from ks_statistic and activity
projection = ["anchor_angle_smoothing_fraction", "pilivar"]
p1, p2 = projection
xlim = (0,1)
_p1distrib = accept["ahat.estimate"][p1]
fig = plt.figure(figsize=(5,5))
ax= sns.histplot(_p1distrib, binrange=xlim)
ax.axvline(0.0625)
print('anchor estimate 1', np.mean(_p1distrib))

_p1distrib = accept["fanjin.top.ks_statistic"][p1]
fig = plt.figure(figsize=(5,5))
ax= sns.histplot(_p1distrib, binrange=xlim)
ax.axvline(0.0625)
print('anchor estimate 2', np.mean(_p1distrib))
```

```
anchor estimate 1 0.1170436586856583
anchor estimate 2 0.22103943483483832
```





[15]:
```
# based on sobol, project this dataset onto pilivar/anchor and do
# rejection ABC to obtain posterior distribution
N = 200
objective = "ahat.estimate"
projection = ["anchor_angle_smoothing_fraction", "pilivar"]
# params[projection+"ahat.estimate"]

statdf = params[parnames+[objective]]
postactive = rejection_abc(statdf, ["ahat.estimate"], reference, N)
# ahat_accepted = postactive[projection+["score"]]
```

```
['ahat.estimate']
(9999, 1)
['ahat.estimate']
N = 200, delta = 0.011243760546231815, target = [0.08248354]
```

```
/home/dan/usb_twitching/pili/src/analysis/abcimplement.py:129:
SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead
```

```
See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  statdf["score"] = score
```

[16]:

```python
# plot the rejection_abc for activity statistic for each subset of the data
def plot_activity(par_accepted, projection, problem):
    parnames = problem["names"]
    fig, axes = plt.subplots(1,2,figsize=(10,5))
    ax1, ax2 = axes
    x, y = projection
    ix, iy = [parnames.index(name) for name in projection]
    sns.set(rc={'figure.figsize':(5,5)})
    ax1 = sns.scatterplot(data=par_accepted, x=x, y=y, hue="score", ax=ax1)
    ax1.set_xlim(bounds[ix])
    ax1.set_ylim(bounds[iy])
    #
    X, Y = par_accepted[x], par_accepted[y]
    ax2 = sns.kdeplot(X,Y, fill=True, ax=ax2)
    ax2.set_xlim(bounds[ix])
    ax2.set_ylim(bounds[iy])
    return fig, axes

N = 200
for i, subset in enumerate(subsets):
    _reference = refdf.iloc[i]
    statdf = params[parnames+[objective]]
    post = rejection_abc(statdf, ["ahat.estimate"], _reference, N)
    ahat_accepted = post[projection+["score"]]
    fig, axes = plot_activity(ahat_accepted, projection, problem)
    fig.suptitle(subset)
```

```
['ahat.estimate']
(9999, 1)
['ahat.estimate']
N = 200, delta = 0.008758155595260234, target = [0.10862537]
```

```
/usr/local/lib/python3.8/dist-packages/seaborn/_decorators.py:36: FutureWarning:
Pass the following variable as a keyword arg: y. From version 0.12, the only
valid positional argument will be `data`, and passing other arguments without an
explicit keyword will result in an error or misinterpretation.
  warnings.warn(
```

```
['ahat.estimate']
(9999, 1)
['ahat.estimate']
N = 200, delta = 0.011243760546231815, target = [0.08248354]
```

```
/home/dan/usb_twitching/pili/src/analysis/abcimplement.py:129:
```

```
SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  statdf["score"] = score
/usr/local/lib/python3.8/dist-packages/seaborn/_decorators.py:36: FutureWarning:
Pass the following variable as a keyword arg: y. From version 0.12, the only
valid positional argument will be `data`, and passing other arguments without an
explicit keyword will result in an error or misinterpretation.
  warnings.warn(
```

```
['ahat.estimate']
(9999, 1)
['ahat.estimate']
N = 200, delta = 0.03603170945224269, target = [0.03630491]
```

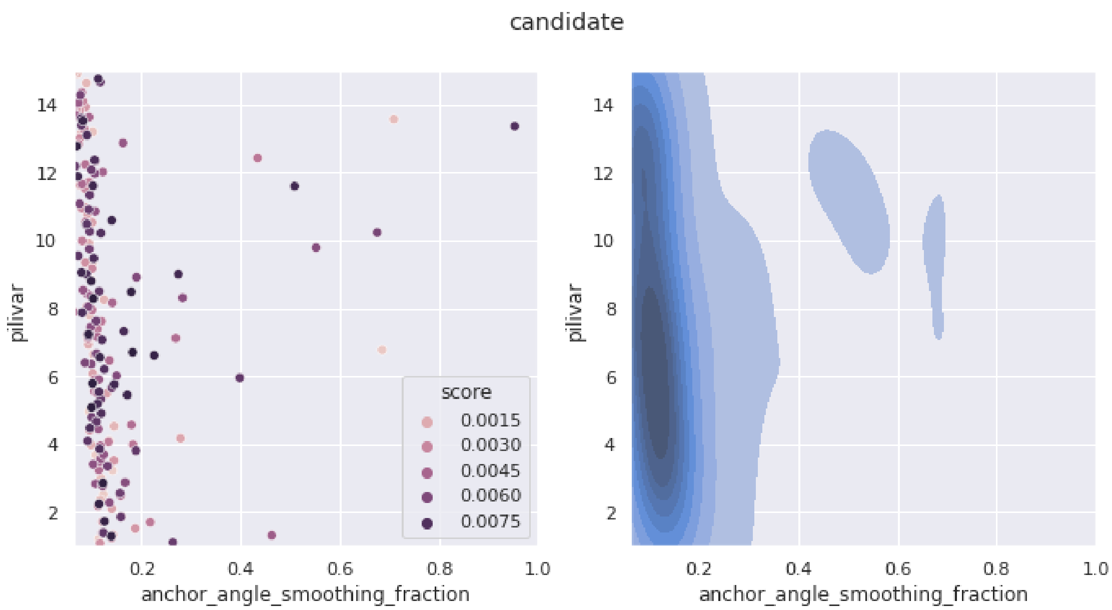
```
/home/dan/usb_twitching/pili/src/analysis/abcimplement.py:129:
SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  statdf["score"] = score
```

```
['ahat.estimate']
(9999, 1)
['ahat.estimate']
N = 200, delta = 0.038368728540705624, target = [0.03396789]
```

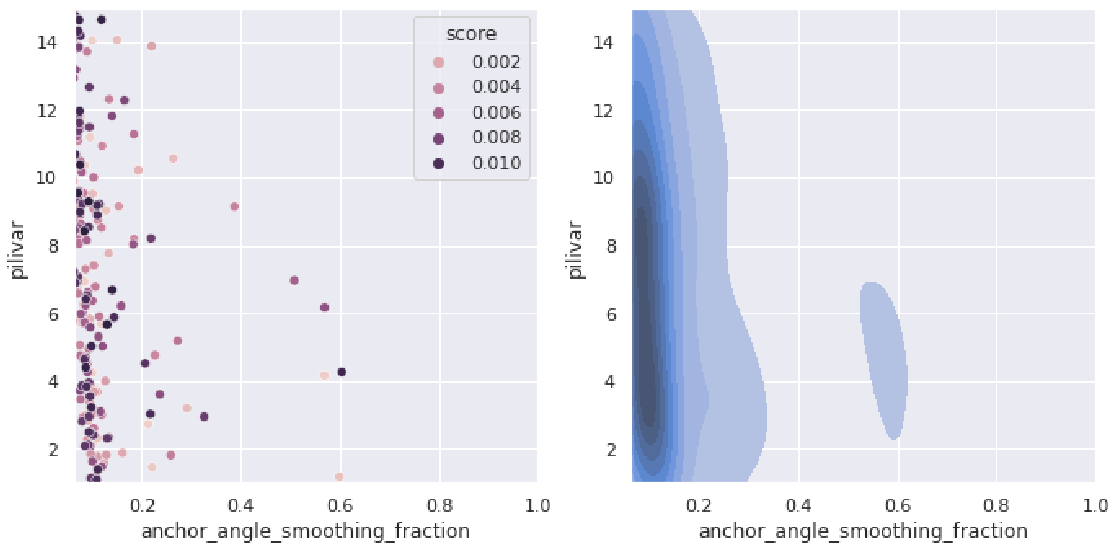
```
/usr/local/lib/python3.8/dist-packages/seaborn/_decorators.py:36: FutureWarning:
Pass the following variable as a keyword arg: y. From version 0.12, the only
valid positional argument will be `data`, and passing other arguments without an
explicit keyword will result in an error or misinterpretation.
  warnings.warn(
/home/dan/usb_twitching/pili/src/analysis/abcimplement.py:129:
SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  statdf["score"] = score
/usr/local/lib/python3.8/dist-packages/seaborn/_decorators.py:36: FutureWarning:
Pass the following variable as a keyword arg: y. From version 0.12, the only
valid positional argument will be `data`, and passing other arguments without an
explicit keyword will result in an error or misinterpretation.
  warnings.warn(
```

```
['ahat.estimate']
(9999, 1)
['ahat.estimate']
N = 200, delta = 0.21031894247241167, target = [0.6371117]
```

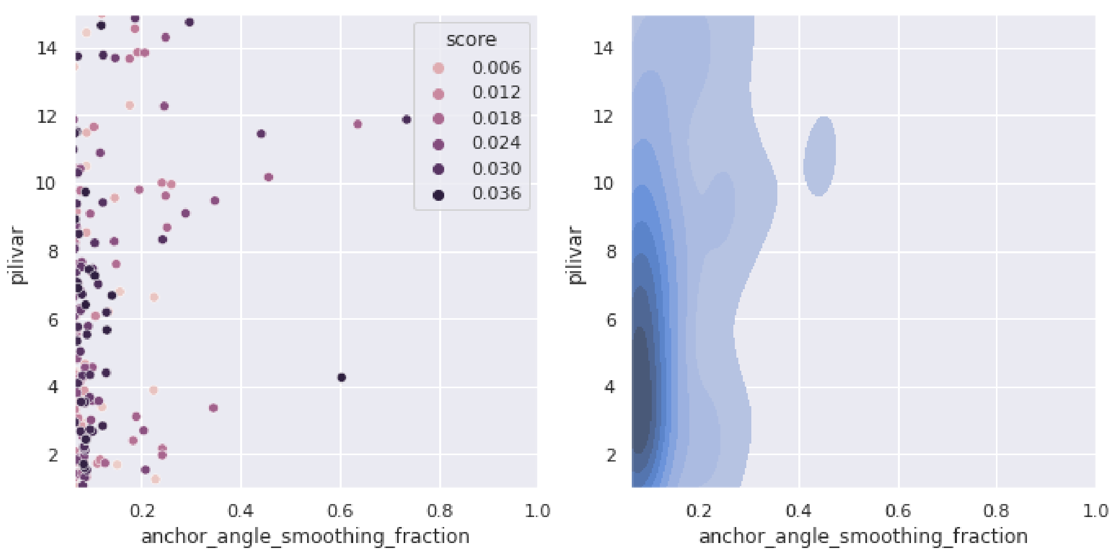
```
/home/dan/usb_twitching/pili/src/analysis/abcimplement.py:129:
SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  statdf["score"] = score
/usr/local/lib/python3.8/dist-packages/seaborn/_decorators.py:36: FutureWarning:
Pass the following variable as a keyword arg: y. From version 0.12, the only
valid positional argument will be `data`, and passing other arguments without an
explicit keyword will result in an error or misinterpretation.
  warnings.warn(
```

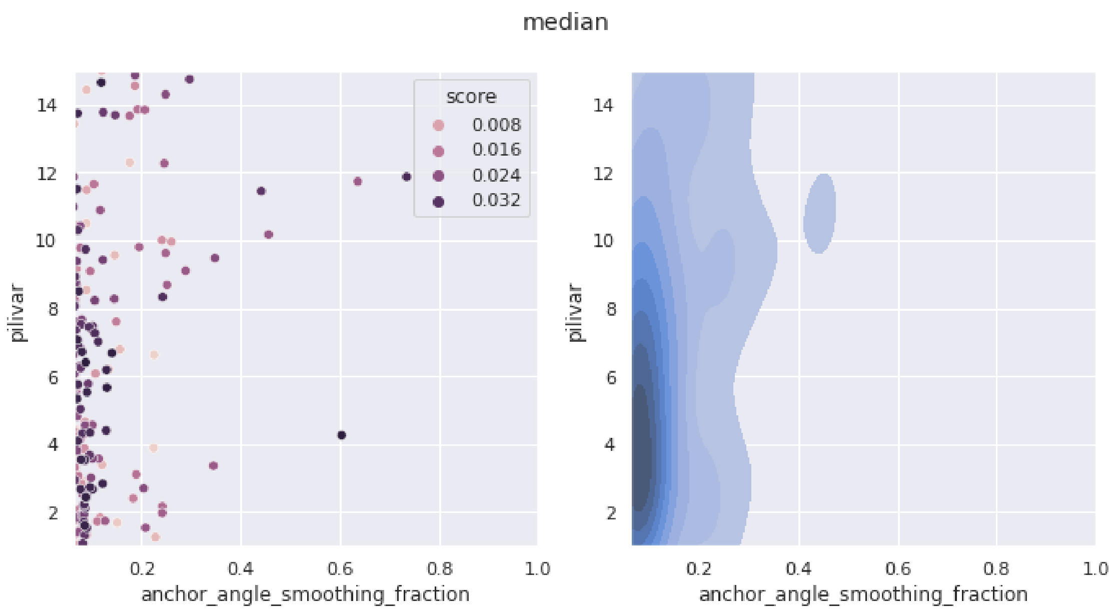


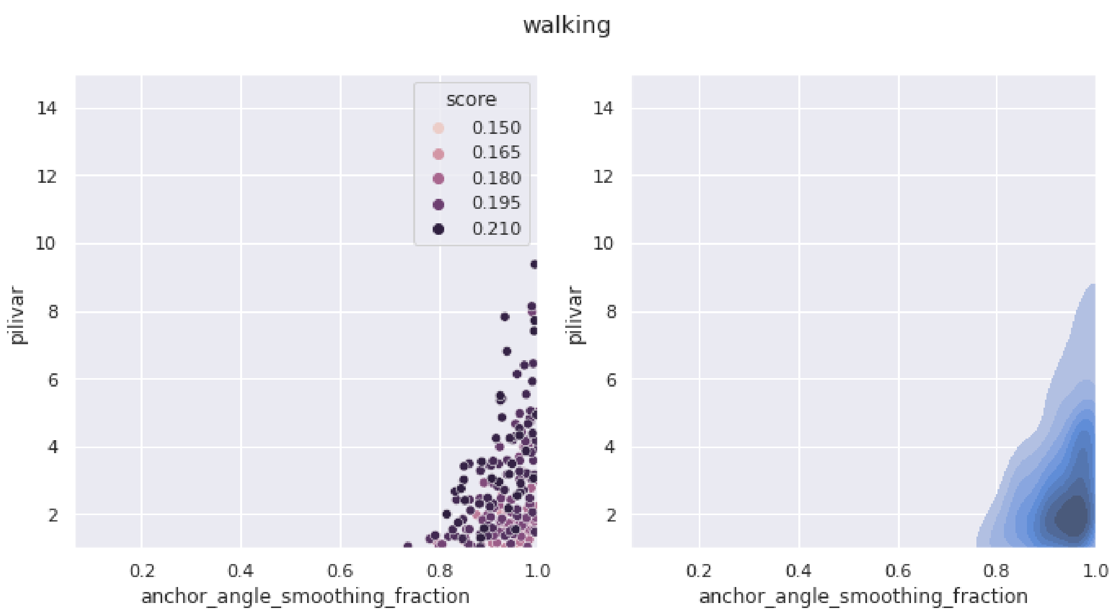
top


score
0.002
0.004
0.006
0.008
0.010
pilivar
anchor_angle_smoothing_fraction
pilivar
anchor_angle_smoothing_fraction

half


score
0.006
0.012
0.018
0.024
0.030
0.036
pilivar
anchor_angle_smoothing_fraction
pilivar
anchor_angle_smoothing_fraction





The shape of the kernel is not that important but the bandwidth is very important.

[17]:
```
# --------------------------------------------------------------------------------
# --------------------------------------------------------------------------------
# TODO move kernel study to a different note book ... (?)
```

```
# # plot the 1d projection of the distribution onto anchor parameter
# # so that we can test sklearn kernel selection
# anchor_parameter = projection[0]
# activitydf = accept["ahat.estimate"]
# activity = activitydf[anchor_parameter].to_numpy()
# sns.histplot(activity, binrange=(0,1.0))
```

[18]:
```
# statsmodels is easier to use than sklearn and gives similar results
use_sklearn = False
if use_sklearn:
    # https://scikit-learn.org/stable/modules/density.html
    # https://jakevdp.github.io/blog/2013/12/01/kernel-density-estimation/
    x = activity
    from sklearn.neighbors import KernelDensity
    from sklearn.model_selection import GridSearchCV
    # https://scikit-learn.org/stable/modules/grid_search.html#grid-search
    import warnings
    # warnings.filterwarnings("ignore", category=UserWarning)
    # warnings.filterwarnings("ignore")
    # some global structure to allow use to both set bandwidths and let them be␣
 ↪estimated
    bw_space_res = 40
    bw_settings = {
        "pilivar": {
            "estimate": True,
            "set": 5.0,
            "geom": np.geomspace(0.1,10.0,bw_space_res)
            },
        "anchor_angle_smoothing_fraction": {
            "estimate": True,
            "set": 0.01,
            "geom":np.geomspace(0.001,0.5,bw_space_res)
            },
        }
    # allow the notebook to vary this
    mod_bw_settings = copy.deepcopy(bw_settings)

def bandwidth_xvalidate(x, bw_space=None, bounds=None, mirror_boundaries=True):
    if mirror_boundaries:
        _x = mirror(x, bounds)
    else:
        _x = x
    if bw_space is None:
        bw_space = np.linspace(np.std(x)/2, (np.max(x)-np.min(x))/2, num=20)
    print("searching bw in range ", bw_space[0], bw_space[-1])
    grid = GridSearchCV(KernelDensity(kernel="epanechnikov"),
```

```
                        {'bandwidth': bw_space},
                        cv=20) # 20-fold cross-validation
    grid.fit(_x[:, None])
    return grid

def kernel_pdf(par_accepted, xlim, bw_space=None, estimate_bandwidth=True,␣
 ↪mirror_boundaries=True):
    x_grid = np.linspace(xlim[0], xlim[1], 200)
    #
    if estimate_bandwidth:
        grid = bandwidth_xvalidate(par_accepted, bw_space=bw_space, bounds=xlim,
            mirror_boundaries=mirror_boundaries)
        print("best", grid.best_params_['bandwidth'])
        kde = grid.best_estimator_
    #
    else:
        if mirror_boundaries:
            par_accepted = mirror(par_accepted, xlim)
        bw = bw_space
        print("set bandwidth", bw)
        kde = KernelDensity(kernel='epanechnikov', bandwidth=bw)
        kde.fit(par_accepted[:, None])
    #
    pdf = np.exp(kde.score_samples(x_grid[:, None]))
    if mirror_boundaries:
        pdf *= 3
    return x_grid, pdf, kde.bandwidth

if use_sklearn:
    estimate_bandwidth = True
    mirror_boundaries = True
    for par in projection:
        print("projection axis ", par)
        ix = parnames.index(par)
        par_accepted = accept["ahat.estimate"][par].to_numpy()
        xlim = problem["bounds"][ix]
        bw_setting = bw_settings[par]
        estimate = bw_setting["estimate"]
        bw_space = bw_setting["geom"] if estimate else bw_setting["set"]
        x_grid, pdf, bandwidth = kernel_pdf(par_accepted.copy(), xlim,␣
 ↪bw_space=bw_space,
            estimate_bandwidth=bw_setting["estimate"], mirror_boundaries=False)
        x_grid, m_pdf, m_bandwidth = kernel_pdf(par_accepted.copy(), xlim,␣
 ↪bw_space=bw_space,
            estimate_bandwidth=bw_setting["estimate"], mirror_boundaries=True)
        mod_bw_settings[par]["set"] = m_bandwidth
```

```
        fig, ax = plt.subplots()
        ax.plot(x_grid, pdf, linewidth=3, alpha=0.5, label='bw=%.4f' %␣
↪bandwidth)
        ax.plot(x_grid, m_pdf, linewidth=3, alpha=0.5, label='mirror bw=%.4f' %␣
↪m_bandwidth)
        ax.set_ylim(bottom=0.0)
        ax.legend(loc='lower right')
        ax.set_title(par)
        plt.show()
```

[19]:

```
# tryout statsmodels for multivariate KDE
import statsmodels.api as sm
ix, iy = [parnames.index(name) for name in projection]
acc = accept["ahat.estimate"]
data = [acc[par].to_numpy() for par in projection]
bw_estimate = sm.nonparametric.KDEMultivariate(data=data, var_type='cc',
    bw='cv_ls')

# mirror the data in the yaxis at the top and bottom
m_data = mirrorpts(data, bounds[iy])
dens = sm.nonparametric.KDEMultivariate(data=m_data, var_type='cc',
    bw='normal_reference')
# use bandwidth estimate from un-mirrored data
dens.bw = bw_estimate.bw
print("statsmodels least squares cross validation bandwidth estimate")
print("bw", dens.bw)
```

```
statsmodels least squares cross validation bandwidth estimate
bw [0.00545344 0.49740232]
```

[20]:

```
# setup control parameters and grid
N = 200
res = 100
ss = ["ahat.estimate"]
projection = ["anchor_angle_smoothing_fraction", "pilivar"]
ix, iy = [parnames.index(par) for par in projection]
xlim, ylim = bounds[ix], bounds[iy]
anchor =  np.linspace(*xlim, num=res)
pilivar =  np.linspace(*ylim, num=res)
pardata = [anchor, pilivar]
```

[21]:

```
# accepted = rejection_abc(statdf, [objective], reference, N)
    # statdf = params[parnames+[objective]]
statdf, statref = abcimplement.regularise_stats(params, reference, objectives)
_acc = rejection_abc(statdf, ss, reference, N, ss_component=True)
```

```
0.0702688796044588
```

```
0.31113147275630193
0.1343752361814738
0.09403116839649117
['ahat.estimate']
(9999, 1)
['ahat.estimate']
N = 200, delta = 0.6867998723053954, target = [0.08248354]
```

[22]:
```
llacc = abcimplement.llregression(_acc, reference, ss, projection)
llacc
```

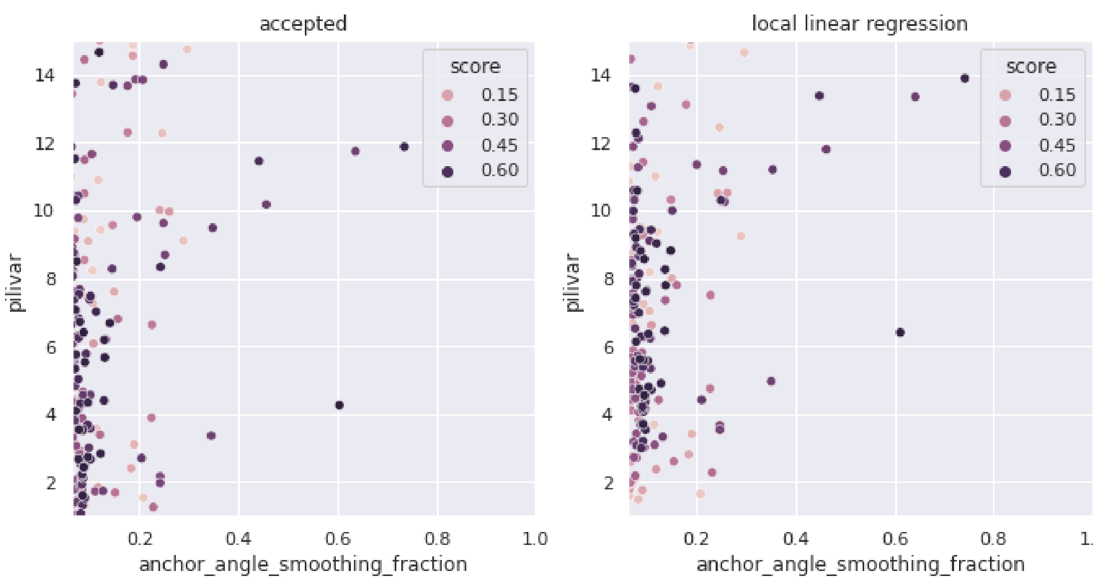
```
max accepted 0.6867998723053954
```

[22]:
```
               uid  dwell_time    pilivar  anchor_angle_smoothing_fraction  \
2472  _u_xoqEd7C3    0.051843  14.841108                         0.186998
6412  _u_0HY54kBH    0.109368   8.181909                         0.105588
6338  _u_39zWeqzJ    0.321406   1.892291                         0.068584
6648  _u_rCKdKQjh    0.053591   9.358616                         0.121576
2332  _u_FQ9rIHh7    0.097793   9.284087                         0.068707
…             …         …         …                              …
5165  _u_1jB4OxuS    0.183448   7.790057                         0.137544
1568  _u_sTRb6oMa    0.178577   8.807350                         0.147882
7081  _u_PRRN2Hff    0.161297  16.769520                         0.125993
96    _u_JylRuSZN    0.051948   6.405316                         0.611389
8396  _u_1skeP91f    0.482870   8.559446                         0.094662

       k_spawn  lvel.mean  deviation.var  qhat.estimate  ahat.estimate  \
2472  1.719385   0.029671       0.194284       1.336925       0.078330
6412  0.760119   0.024629       0.376570       0.943546       0.067279
6338  0.969261   0.043197       1.233796       1.047862       0.100282
6648  3.170234   0.061444       0.274346       3.139049       0.063620
2332  2.825736   0.037825       0.256784       2.284099       0.052340
…          …         …            …             …             …
5165  5.083550   0.357931       0.570342       2.156662       0.760338
1568  1.045740   0.082371       0.508090       0.628456       0.761220
7081  2.684515   0.074493       0.276509       0.670180       0.762083
96    2.086445   0.173446       0.936012       0.596596       0.766300
8396  6.604770   0.380821       0.489364       2.145791       0.769283

         score        s0    weight
2472  0.004153 -0.004153  1.091981
6412  0.015205 -0.015205  1.091486
6338  0.017798  0.017798  1.091288
6648  0.018864 -0.018864  1.091197
2332  0.030143 -0.030143  1.089918
…          …         …         …
5165  0.677855  0.677855  0.028261
```

```
1568  0.678737  0.678737  0.025490
7081  0.679599  0.679599  0.022777
96    0.683816  0.683816  0.009468
8396  0.686800  0.686800  0.000000

[200 rows x 12 columns]
```

[23]:
```
# scatter side by side
fig, axes = plt.subplots(1,2,figsize=(10,5))
p1, p2 = projection
#
ax = axes[0]
ax = sns.scatterplot(data=_acc, x=p1, y=p2, hue="score", ax=ax)
ax.set_xlim(bounds[ix])
ax.set_ylim(bounds[iy])
ax.set_title("accepted")
#
ax = axes[1]
ax = sns.scatterplot(data=llacc, x=p1, y=p2, hue="score", ax=ax)
ax.set_xlim(bounds[ix])
ax.set_ylim(bounds[iy])
ax.set_title("local linear regression")
```

[23]:
```
Text(0.5, 1.0, 'local linear regression')
```



[24]:
```
# we implement epanechnikov kernel but scipy.stats.gaussian_kde does a better␣
↪job
# we still use epanechnikov kernel for weighting by summary statistic
```

```
from abcimplement import new_epanechnikov

# Now attempting to implement much more complex beaumont regression ABC
# 1. compute standard deviation of summary statistics
# if we use only one summary statistic does this even matter?
def smooth_regression_abc(problem, params, sstat, reference, projection=None,
    N= 200
    ):
# params dataframe contains parameters and normal summary statistics but not␣
↪lvel similarity statistic
    _names = problem["names"]
    _bounds  = problem["bounds"]
    ix, iy = [_names.index(par) for par in projection]
    xlim, ylim = _bounds[ix], _bounds[iy]

    statdf, statref = abcimplement.regularise_stats(params, reference, sstat)
    _acc = rejection_abc(statdf, sstat, reference, N, ss_component=True)
    _acc = abcimplement.llregression(_acc, reference, sstat, projection)
    weight = _acc["weight"]

    def statsmodels_dens(pardata, res, mirror_yaxis=True):
        # NO WEIGHTS
        data = [_acc[_p].to_numpy() for _p in projection]
        bw_estimate = sm.nonparametric.KDEMultivariate(data=data,␣
↪var_type='cc', bw='cv_ls')
        if mirror_yaxis:
            data = mirrorpts(data, ylim)
        dens = sm.nonparametric.KDEMultivariate(data=data, var_type='cc',
            bw='normal_reference')
        dens.bw = bw_estimate.bw
        print("bw", dens.bw)
        X1, X2 = np.meshgrid(anchor, pilivar)
        result = 3*dens.pdf([X1.ravel(), X2.ravel()])
        _grid = result.reshape([100,100])
        return X1, X2, _grid

    # posterior distibution at parameter
    def gkde_eval_posterior(pardata, res, mirror_yaxis=True):
        # take the accepted parameter data arrays
        #
        anchor, pilivar = pardata
        X1, X2 = np.meshgrid(anchor, pilivar)
        # the accepted parameters
        data = [_acc[_p].to_numpy() for _p in projection]
        _weight = weight
        if mirror_yaxis:
            data = mirrorpts(data, ylim)
```

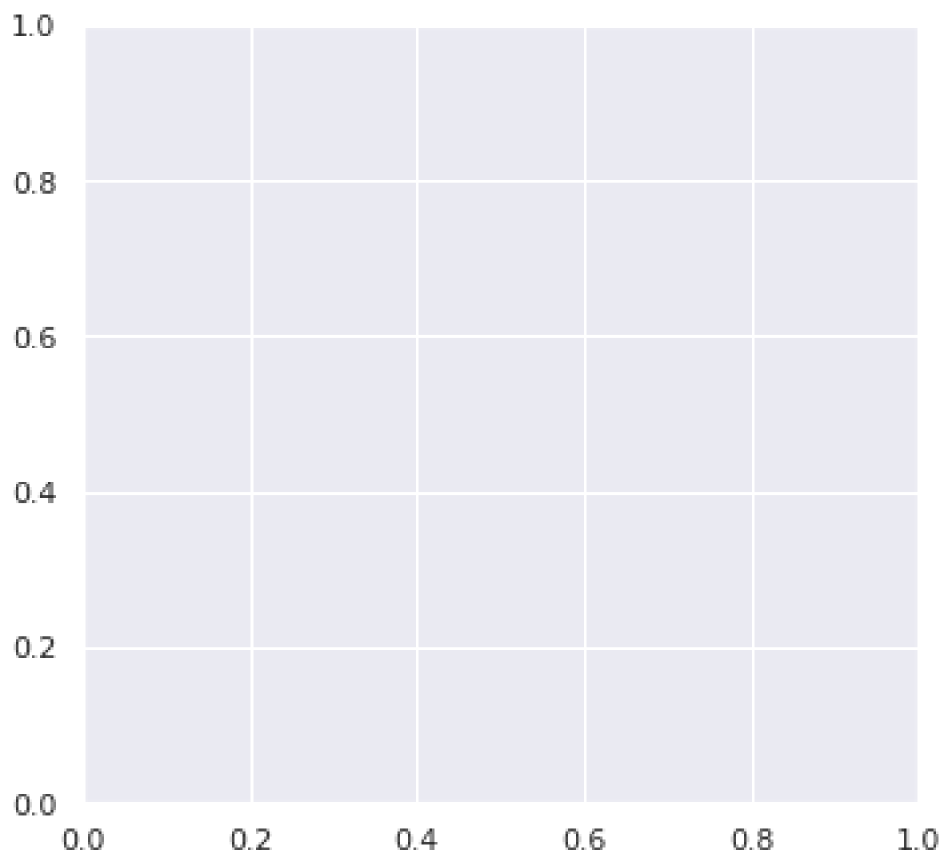
```
            _weight = np.concatenate([weight,weight,weight])
        gkde = scipy.stats.gaussian_kde(np.stack(data),weights=_weight)
        pdf = 3*gkde.evaluate(np.stack([X1.ravel(), X2.ravel()]))
        return X1, X2, pdf.reshape((res,res))

    def eval_posterior(pardata, res, mirror_yaxis=True):
        delta_p1, delta_p2 = bw_estimate.bw
        kern1 = new_epanechnikov(delta_p1)
        kern2 = new_epanechnikov(delta_p2)
        anchor, pilivar = pardata
        X1, X2 = np.meshgrid(anchor, pilivar)
        posterior = np.zeros((len(anchor),len(pilivar)))
        par1, par2 = [_acc[_p].to_numpy() for _p in projection]
        # slow double loop
        for index, anchor_v in np.ndenumerate(X1):
            pilivar_v = X2[index]
            _num = np.array([kern1(par1[i] -anchor_v)*kern2(par2[i] -␣
 ↪pilivar_v) for i in range(N)])
            posterior[index] = np.sum(_num * weight)/np.sum(weight)
        return X1, X2, posterior

    # return gkde_eval_posterior
    # return eval_posterior
    return statsmodels_dens

eval_posterior = smooth_regression_abc(problem, params, ss, reference,
    projection=projection, N=N)
#
X1, X2, posterior = eval_posterior(pardata, res=res)
print("computed posterior")
```

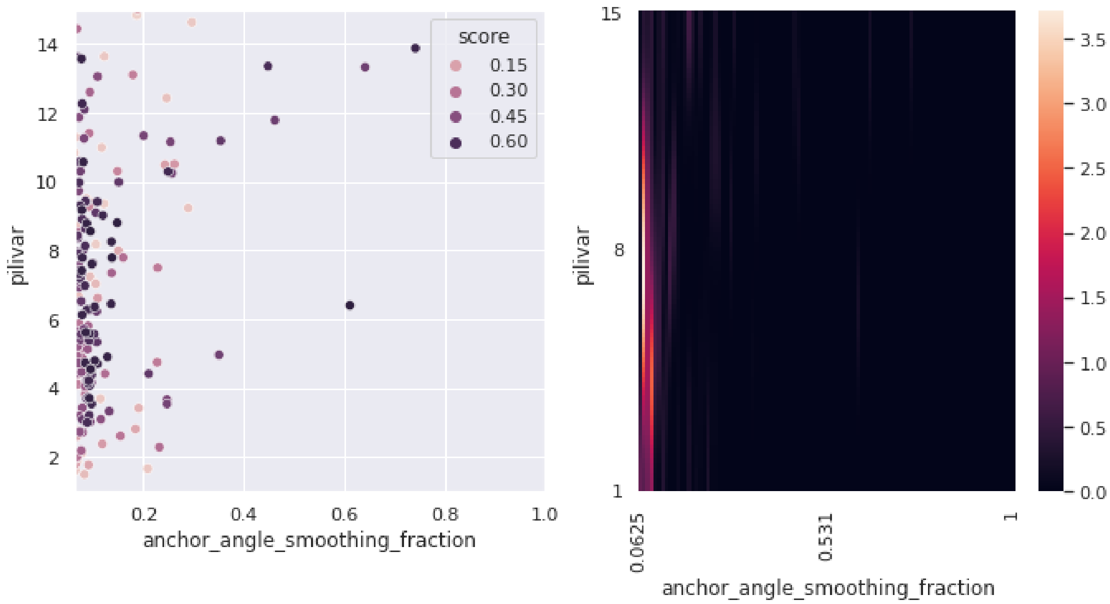
```
0.09403116839649117
['ahat.estimate']
(9999, 1)
['ahat.estimate']
N = 200, delta = 0.6867998723053954, target = [0.08248354]
max accepted 0.6867998723053954
bw [0.00235612 1.62741604]
computed posterior
```

[25]:
```
# palette = sns.color_palette("viridis", as_cmap=True)
fig, ax = plt.subplots()
pdata = pd.DataFrame(posterior, anchor, pilivar)
fig, axes = plt.subplots(1,2,figsize=(10,5))
ax = axes[1]
sns.heatmap(pdata, ax=ax)
_p1, _p2 = projection
```

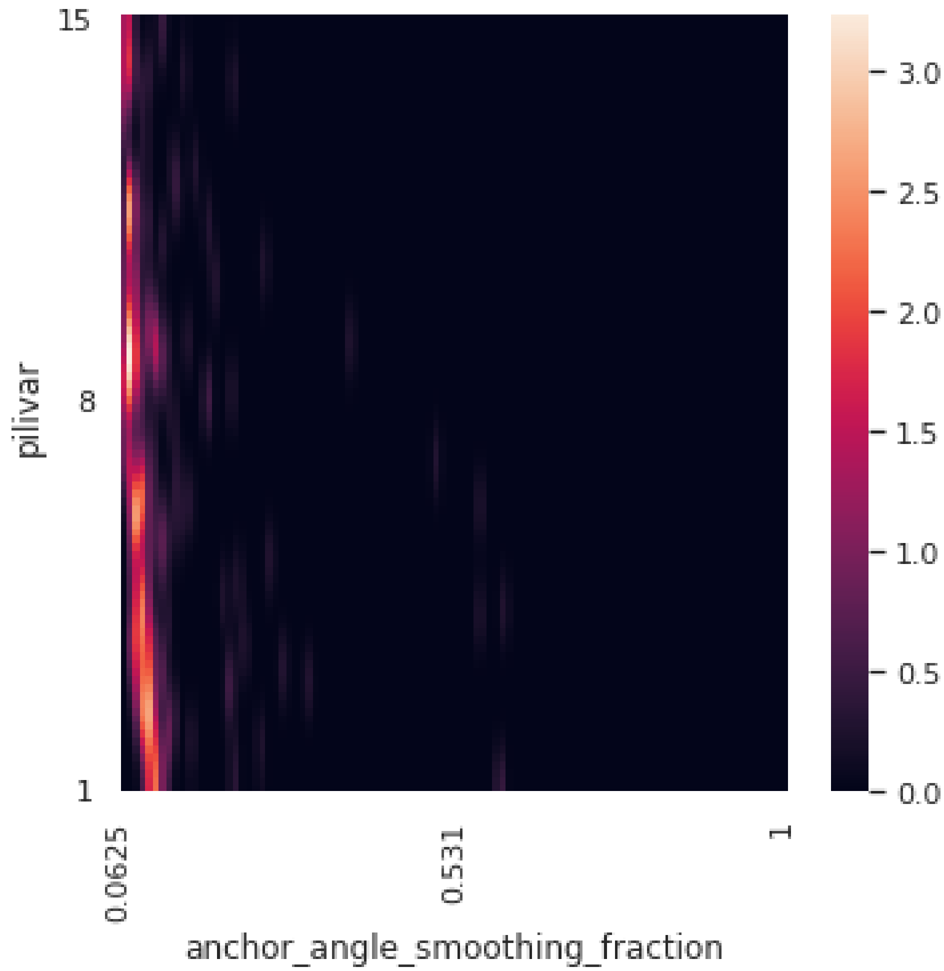
```
def _heatmap_ax(ax, _bounds):
    xlim, ylim = _bounds
    ax.invert_yaxis()
    # simplify this tick locator business
    ax.set_xticks([0,res//2,res-1])
    ax.set_yticks([0,res//2,res-1])
    ax.set_xticklabels(["{:.3g}".format(x) for x in np.linspace(*xlim, num=3,␣
 ↪endpoint=True)])
    ax.set_yticklabels(["{:.3g}".format(x) for x in np.linspace(*ylim, num=3,␣
 ↪endpoint=True)])
    ax.set_xlabel(_p1)
    ax.set_ylabel(_p2)
_heatmap_ax(ax, [xlim, ylim])
# scatter
ax = axes[0]
p1, p2 = projection
ax = sns.scatterplot(data=llacc, x=p1, y=p2, hue="score", ax=ax)
ax.set_xlim(bounds[ix])
ax.set_ylim(bounds[iy])
```

[25]: (1.0, 15.0)





[26]:
```
# Must be after the anchor/pilivar basis is defined
# statsmodels = False
statsmodels = True
if statsmodels:
    X1, X2 = np.meshgrid(anchor, pilivar)
    result = 3*dens.pdf([X1.ravel(), X2.ravel()])
    _grid = result.reshape([100,100])
    ax = sns.heatmap(_grid)
    _heatmap_ax(ax, [xlim, ylim])
```



[27]:
```
# compare bandwidth settings
# print("me", [mod_bw_settings[par]["set"] for par in projection])
# print("statmodels", dens.bw)
# check normalization
# https://coderedirect.com/questions/502920/
↪integrating-2d-samples-on-a-rectangular-grid-using-scipy
check = False
if check: # normalization
    from scipy.integrate import simps
    print("pdf integrates to ", simps(simps(posterior, anchor), pilivar))
    line = np.sum(posterior,axis=0)
    plt.plot(anchor, line)
    estimate1d = np.sum(anchor*line)/np.sum(line)
    print("simple anchor parameter estimate {:.2g}".format(estimate1d))
# we used this estimate to skip ahead and do abc with the anchor parameter␣
↪frozen out
```

```
# see ~/usb_twitching/run/5bfc8b9/cluster/mc3d_frozen
```

[28]:
```
#␣
↪-------------------------------------------------------------------------------
#␣
↪-------------------------------------------------------------------------------
# sampling arbitrary distributions
```

[29]:
```
# sample this pdf
# 1. interpolate to a smooth function
# https://docs.scipy.org/doc/scipy/reference/generated/scipy.interpolate.
↪interp2d.html
# 2. check the interpolation
# 3. sampling
# https://stackoverflow.com/questions/49211126/
↪efficiently-sample-from-arbitrary-multivariate-function
```

[30]:
```
# pinky library does give any better result than our brute force sampling
if verbose:
    # someone has done the work for us so lets use it
    sys.path.append(join(notedir, "lib/pinky"))
    from pinky import Pinky
    ix, iy = [parnames.index(par) for par in projection]
    xlim, ylim = bounds[ix], bounds[iy]
    extent = np.array([*xlim, *ylim])
    print(extent)
    pink = Pinky(P=posterior, extent=extent)
    x0 = np.array([0.2,10.0])
    samples = pink.sample(1000, r=1)
    x, y = samples.T
    ax = sns.kdeplot(x, y, levels=10, fill=True, bw_adjust=0.8)
    ax.set_xlim(xlim)
    ax.set_ylim(ylim)
    ax.set_title("resampled")
```

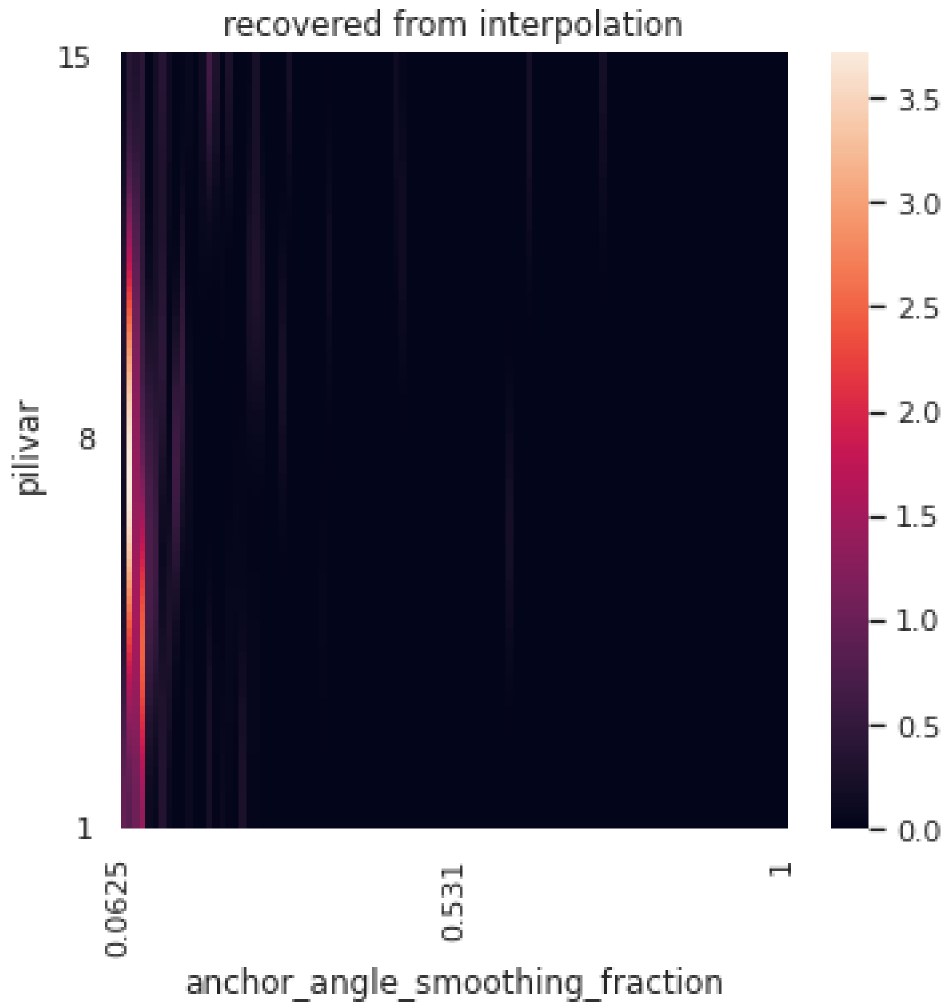
pinky is fast but the sampling doesn't seem all that accurate the denisty tapers the y-boundary and seems unnecessarily smoothed although that could be seaborn.kdeplot

[31]:
```
# for our own sampling implementation we need to interpolate the posterior␣
↪distribution
from numpy.random import uniform
import scipy.interpolate
# image data is stored in numpy row order arrays
# hence the 0th axis in the array is the y axis
# we choose to construct interpolated functions which accept (y,x) as arguments␣
↪rather than (x,y)
bbox = [*ylim, *xlim]
```

```
print("bbox", bbox)
# For whatever reason scipy recommends RectBivariateSpline for rectangular␣
↪samples. Lets trust them.
target_density = scipy.interpolate.
↪RectBivariateSpline(pardata[1],pardata[0],posterior,
    bbox=bbox)

# test the interpolation
show = np.zeros(posterior.shape)
for index, x in np.ndenumerate(X1):
    y = X2[index]
    show[index]  = target_density(y,x)
ax = sns.heatmap(show)
_heatmap_ax(ax, [xlim,ylim])
ax.set_title("recovered from interpolation")
# its good
```

```
bbox [1.0, 15.0, 0.0625, 1.0]
```

[31]: Text(0.5, 1.0, 'recovered from interpolation')



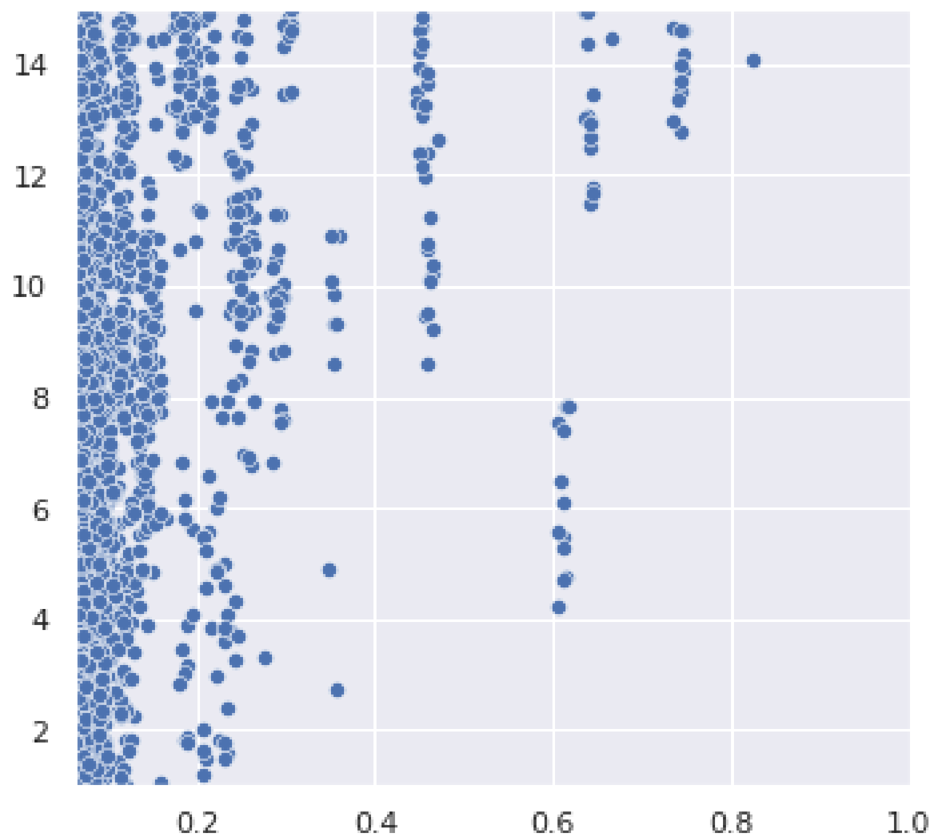
[32]:

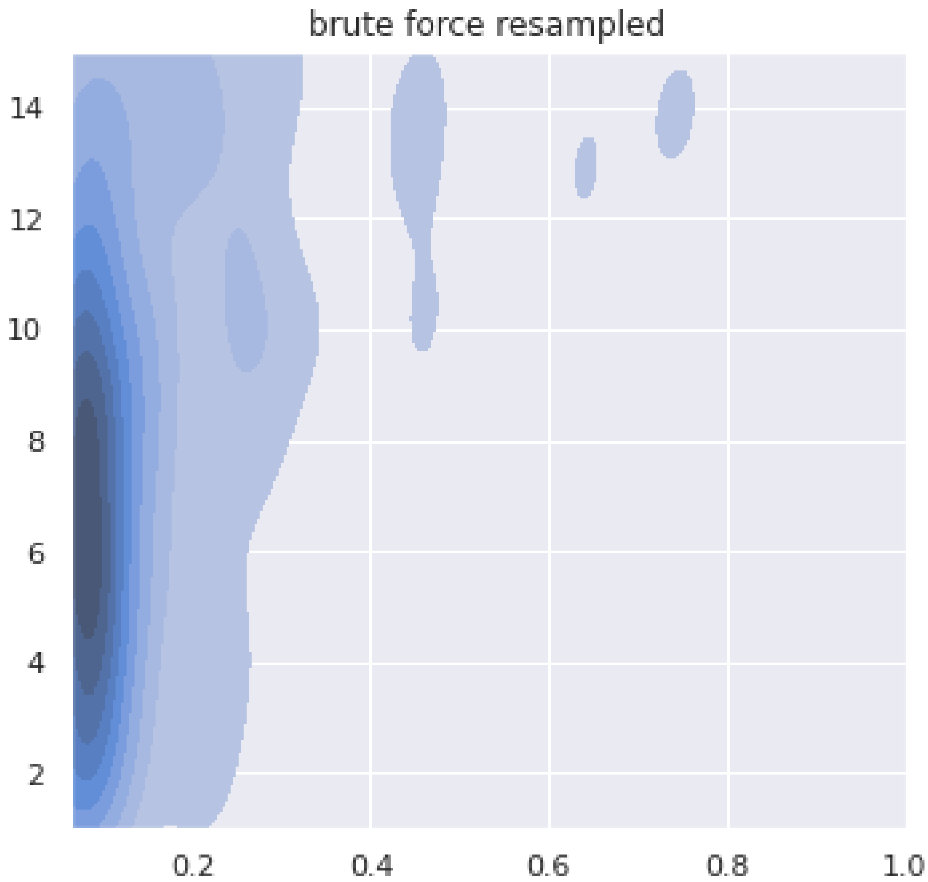
```
# test our brute force sampling
from abcimplement import force_sample_target

# maximum (from sampled pdf)
zlim = (0, np.max(posterior))
xt, yt = force_sample_target(target_density, [xlim, ylim, zlim])
print("nsamples", len(xt))
fig, ax = plt.subplots()
ax  = sns.scatterplot(x=xt,y=yt)
ax.set_xlim(*xlim)
ax.set_ylim(*ylim)
fig, ax = plt.subplots()
ax = sns.kdeplot(xt,yt, fill=True, ax=ax)
ax.set_xlim(*xlim)
ax.set_ylim(*ylim)
```

```
ax.set_title("brute force resampled")
# works well
```

```
nsamples 1979

/usr/local/lib/python3.8/dist-packages/seaborn/_decorators.py:36: FutureWarning:
Pass the following variable as a keyword arg: y. From version 0.12, the only
valid positional argument will be `data`, and passing other arguments without an
explicit keyword will result in an error or misinterpretation.
  warnings.warn(
```

[32]: Text(0.5, 1.0, 'brute force resampled')





[33]:
```
# ------------------------------------------------------------------
# ------------------------------------------------------------------
# mc3d with fixed anchor parameter = 0.17
# see rejectionabc.py
```